

SIMULATION OF A PROCESS PLANT FOR PRODUCTION OF BENZENE, TOLUENE AND XYLENE FROM LIQUIFIED PETROLEUM GAS

U.S. Ubam, U.D. Amoka and I. Shaibu

Chemical Engineering Department, Ahmadu Bello University, Zaria-Nigeria

Correspondence: ubam75@gmail.com, 07068876231

ABSTRACT

Liquified petroleum gas (LPG) are promising feedstock for production of high purity petrochemicals as they are relatively cheap and readily available. LPG feedstock is subjected to ASPEN simulation to generate the petrochemicals benzene, toluene and xylene. Benzene, toluene and xylene (BTX) were produced via simulation from propane and butane (LPG) using the ASPEN HYSYS simulation package. The purity level of 68.83% benzene, 89% toluene and 92% xylene were obtained from the product upgrading processes at feed composition level of 80% propane and 20% butane. Power requirement of 5.33 MW was obtained from the overall energy balance of the process using the ASPEN energy analyzer. The work shows a complete model of a plant that yielded high purity BTX from LPG.

Keyword: LPG, BTX, ASPEN simulation

1 INTRODUCTION

The production of several chemicals required for other processes are dependent on the raw material intermediates. Benzene, toluene and xylene (BTX) are aromatic hydrocarbons which are desired species for the synthesis of chemicals (other petrochemicals) such as styrene, phenol, polyurethane, phthalic anhydrides etc. they can also be used as solvents in the production of paints and other valuable products [1]. Nigeria is number one crude oil exporters in Africa due to its abundant reserves [2]. Petrochemical based product depend on crude oil distillates and natural gas for their synthesis [3]. Feedstock for BTX production in Nigeria and most part of the world are obtained through the catalytic reforming of naphtha resulting to higher octane reformat and few percentage of BTX [4]. Huge amount of money will be saved from importation of BTX if a process plant for its production is incorporated in Nigeria.

BTX are primarily produced by the catalytic reforming of naphtha over H-ZSM-5 via the cyclor process. However, the product from the catalytic reforming of naphtha contains about 10-15% benzene, 50-55% of toluene and 30-35% of xylene [4]. The work carried out by Mukhtar in 2016 on simulation of LPG aromatization to BTX shows that propane and butane are desired feedstock for BTX synthesis [5], but the simulation entails three plug flow reactors

producing 21% benzene, 5% toluene and 5% xylene. However, the cost of three plug flow reactors giving rise to smaller yield of BTX renders the design invalid.

The cost for naphtha to liquified petroleum gas (LPG) is a concerning issue as naphtha feedstock cost about \$590 per ton [2], while propane cost about \$295 per ton and \$330 per ton for butane [6]. On the other hand, lower alkane tend to give better conversion of BTX compared to longer chain alkane [4].

The mechanism of reaction is as thus; propane and butane form their respective alkenes through dehydrogenation reaction which is the rate limiting step of the overall reactions occurring. Longer chain hydrocarbons are formed from the oligomerization of alkenes which thereby form naphthenes before dehydrogenation occur to form aromatics. Excessive hydrogen formation due to the above process makes the process to become strongly endothermic and as such, recycling of hydrogen back to the reactor to reduce coking and catalyst sintering is required. However, from the overall known mechanisms, only two stoichiometric equation for the conversion of propane and butane to BTX are known as no information on the actual kinetic equations was found [7]. Because of the endothermic nature of the process, temperature of 500⁰C is required to activate the reaction [8].

Advanced System for Process Engineering (ASPEN) Hyprotech System (HYSYS) is a strong engineering tool that is used in the industries for research, development, design and modelling of chemical engineering processes [9][10]. This research is aimed at producing BTX from LPG using steady state simulation ASPEN HYSYS.

2 MATERIALS AND METHODS

2.1 Property Set

The simulation was carried out using ASPEN HYSYS. Table 1 shows the components used. The Peng Robinson equation of state was selected as the fluid package and all kinetic reactions involved were added. Table 2 shows the kinetic reactions for the aromatization steps involved. The overall energy balance, power requirement and utility formulations were obtained from ASPEN energy analyzer.

2.2 Simulation Environment

The feed material stream containing 80 kmol/hr of propane and 20 kmol/hr of butane at 150 ⁰C and 120 kPa was heated to 500 ⁰C and sent to a conversion reactor. The effluent was cooled and flashed to separate the very light vapour from the heavier liquid. The vapour was compressed and cooled in order to further separate the natural gas from the hydrogen. The bottom of the separator was sent to the distillation column for product upgrading. Benzene was retrieved from column C03 while toluene and xylene were retrieved from column C05 and C06 respectively. Figure 1 shows the process flow diagram (PFD) for the simulated case.

Table 1: Feed Properties

Component name/ Operating conditions	Value
Propane	0.8
Butane	0.2
Temperature (°C)	150
Pressure (kPa)	120
Mass flow (kg/hr)	4690

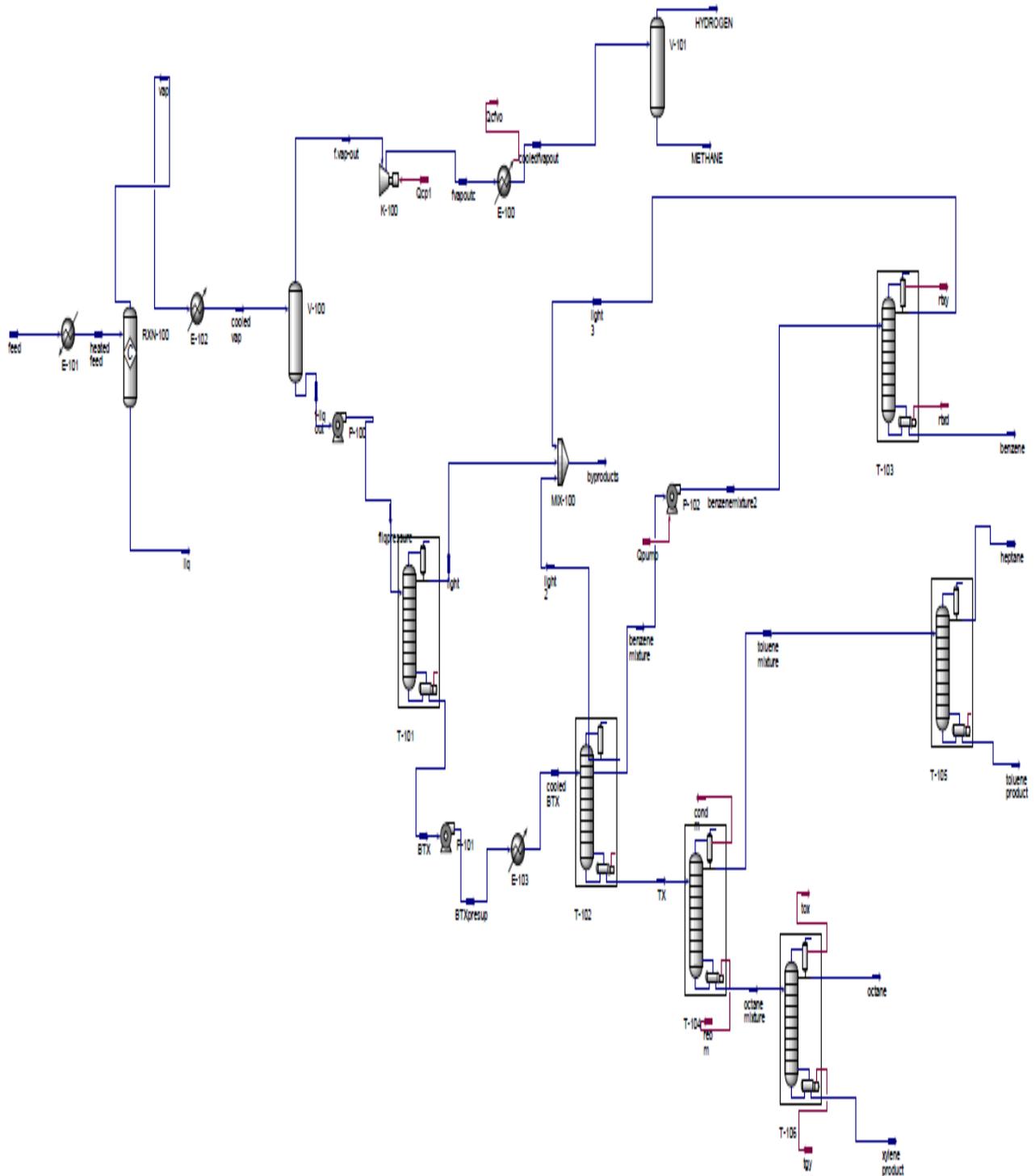


Figure 1. Process flow Diagram

Table 2: Reactions for Aromatization.

Aromatization
$C_6H_{12} + 3 C_2H_4 > B + 3 C_2H_6$
$C_7H_{14} + 3 C_2H_4 > T + 3 C_2H_6$
$C_8H_{16} + 3 C_2H_4 > X + 3 C_2H_6$
$C_6H_{12} + 3 C_3H_6 > B + 3 C_3H_8$
$C_7H_{14} + 3 C_3H_6 > T + 3 C_3H_8$
$C_8H_{16} + 3 C_3H_6 > X + 3 C_3H_8$
$C_6H_{12} + 3 C_4H_8 > B + 3 C_4H_{10}$
$C_7H_{14} + 3 C_4H_8 > T + 3 C_4H_{10}$
$C_8H_{16} + 3 C_4H_8 > X + 3 C_4H_{10}$
$C_6H_{12} + 3 C_5H_{10} > B + 3 C_5H_{12}$
$C_7H_{14} + 3 C_5H_{10} > T + 3 C_5H_{12}$
$C_8H_{16} + 3 C_5H_{10} > X + 3 C_5H_{12}$
$C_6H_{12} + 3 C_6H_{12} > B + 3 C_6H_{14}$
$C_7H_{14} + 3 C_6H_{12} > T + 3 C_6H_{14}$
$C_8H_{16} + 3 C_6H_{12} > X + 3 C_6H_{14}$
$C_6H_{12} + 3 C_7H_{14} > B + 3 C_7H_{16}$
$C_7H_{14} + 3 C_7H_{14} > T + 3 C_7H_{16}$
$C_8H_{16} + 3 C_7H_{14} > X + 3 C_7H_{16}$
$C_6H_{12} + 3 C_8H_{16} > B + 3 C_8H_{18}$
$C_7H_{14} + 3 C_8H_{16} > T + 3 C_8H_{18}$
$C_8H_{16} + 3 C_8H_{16} > X + 3 C_8H_{18}$

3 RESULTS AND DISCUSSION

3.1 Variability Study of Selected Units

3.1.1 Feed composition effect on BTX mole fraction in the reactor

Figure 2 show the fractional conversion of propane to BTX at 500 °C and 125 kPa reaction condition. It can be detected that as mass fraction of propane (C₃) to butane (C₄) increases from 20% to 100%, the yield of benzene increases up to a point where the fraction of propane to butane was 60% to 40%. Toluene and xylene mass fractions were small as C₃ and C₄ mass fractions were increased from 20% to 100% up to a point where the butane fraction was 40% in which an increase in mass fraction was seen. This shows that production of xylene is strongly dependent on the few mass fractions of butane. Figure 2 also shows that to obtain a reasonably BTX conversions, composition level of propane and butane should be between 80% and 20% respectively.

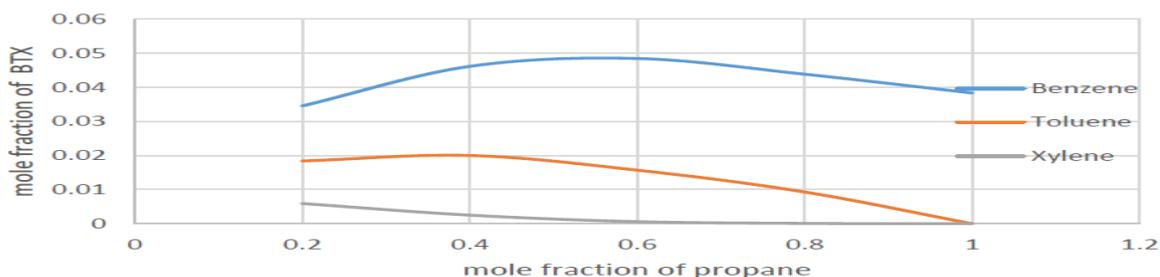


Figure 2. Feed composition effect on BTX mole fraction

3.1.2 Temperature Effect on BTX Formation

Figure 3 shows the temperature effect on BTX formation at 125 kPa constant pressure. Reaction temperature increase from 300-400 °C increases benzene (0.0041-0.0439) and toluene (0.002- 0.0093) yield. However, no xylene yield was seen within the above temperature range. Benzene and toluene yield appreciate up to a temperature of 500 °C and remain constant above that temperature range. However, xylene composition remains constant at temperature of 400 °C and above.

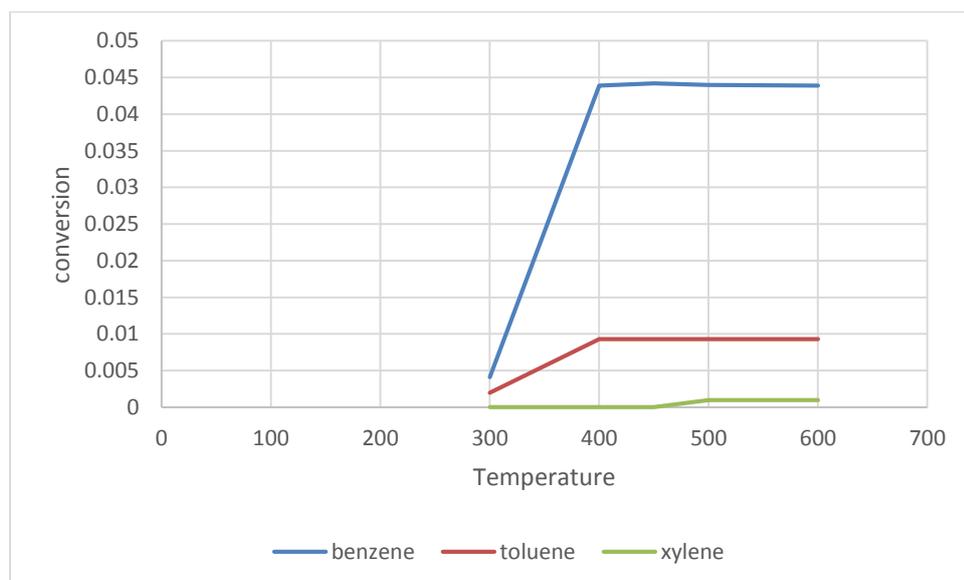


Figure 3. Temperature effect on BTX formation

3.1.3 Pressure Effect on BTX Formation

Figure 4 shows the effect of pressure on BTX formation. It is seen that at a pressure of 125-350 kPa, the composition of BTX remains constant. This could also imply that production of BTX can be carried out at atmospheric pressure.

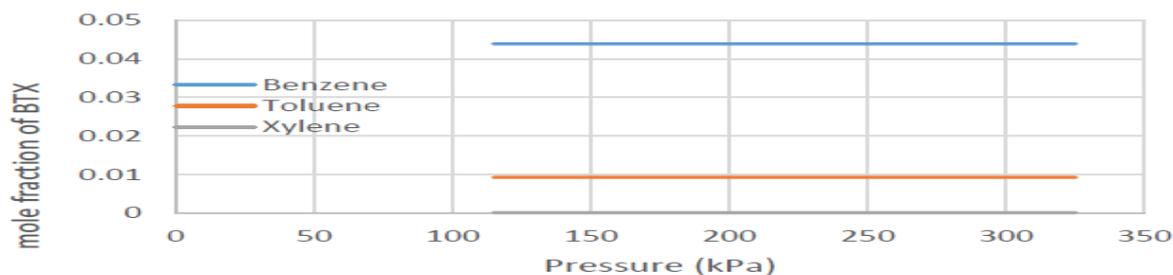


Figure 4. Pressure effect on BTX formation

3.1.4 Effect of Number of Trays on Purity of Benzene, Toluene and Xylene

Figure 5 shows the variation of percentage purity of BTX with number of trays. It can be deduced that purity level of xylene increases rapidly with the number of trays in the column. However, as the number of trays of xylene increases, the distillate becomes more than the bottom product which renders the design invalid if larger volume of product is not produced. Factors such as reflux ratio and mass rate on column design specification has to be altered. A percentage purity of 91% was obtained as the reflux ratio was increased to 20 and mass rate of the top product reduced to 21.5 kg/hr. This assist in reducing the amount of heptane produced and increasing the amount of xylene.

In comparison to xylene, toluene purity does not increase appreciably with the number of trays at constant temperature and pressure. From the simulation obtained, the optimum tray number for toluene is 40 trays with only about 1% purity increase from 30 to 40 trays. Additional trays in the column will only add up to the cost of production.

Purity level of benzene is not solely affected by the number of trays. It can be seen that the purity is constant from 30-60 trays. Only a small increase of 0.05 was observed with additional 10 trays from 20-30. Therefore, the purity level in benzene column is not primely affected by the number of trays and as such, more trays will only incorporate more cost.

The purity level against the tray number of BTX shows that the purity of lighter petrochemicals (benzene and toluene) will not readily increase. This might be due to the molecular structure of benzene and toluene as xylene which is higher in molecular weight will have a better purity to the former. From the simulation, higher molecular weight petrochemicals will tend to have better purity with respect to tray number than the lower ones.

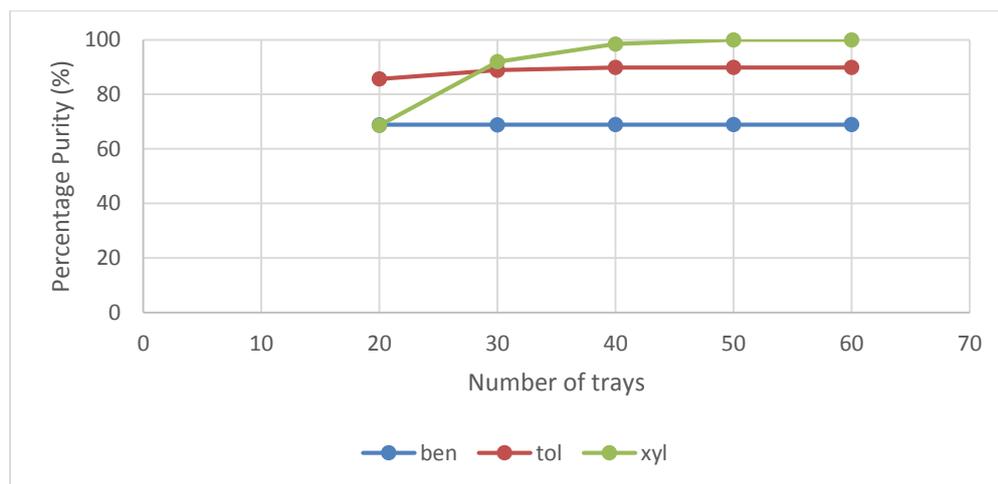


Figure 5. Variation of percentage purity of BTX with number of trays

3.2 Energy Requirement and Utilities

3.2.1 Energy Requirements

Figure 8 present the overall heating and cooling processes in the BTX plant as calculated by the ASPEN Energy analyzer. The energy balance for overall heating process was 9.704×10^6 kJ/hr and 9.496×10^6 kJ/hr for cooling respectively. The total energy balance was 19.2×10^6 kJ/hr which is equivalent to 5.33 MW. This implies that, there is high demand for energy in the overall production of BTX.

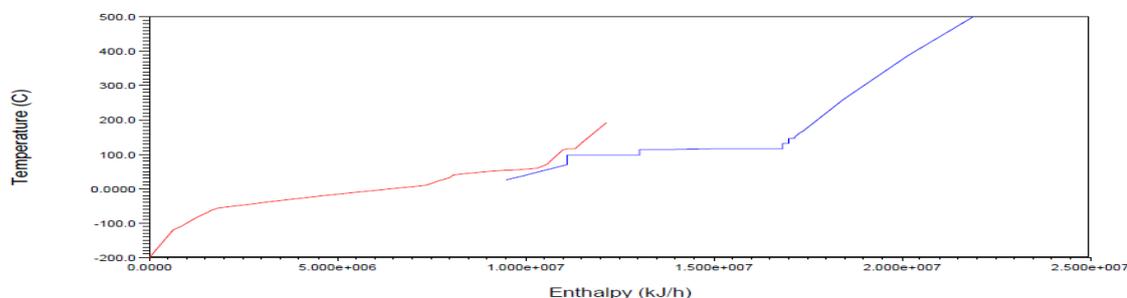


Figure 6. Enthalpy against temperature curve of the simulated BTX plant.

3.2.2 Utilities

Table 3 present the overall process utilities required for the BTX production plant as analysed by the ASPEN energy analyzer. It can be seen that steam generations (high, low and medium pressure steams) and refrigerating of products (BTX) and some by-products (hydrogen and methane) consumes the highest amount of energy and therefore offers very high heat transfer coefficient. This is due to physical properties like the boiling point in which the products exist; most of which have boiling points at ultimate negative temperatures.

Table 3. Overall Utilities for unit operations

Utility Database							
Name	Type	Inlet T (C)	Outlet T (C)	HTC (kJ/h-m ² -C)	Cost Index (Cost/kJ)	ARH (C)	ARL (C)
LP Steam	HOT	125.0 *	124.0 *	21600.00 *	1.900e-006 *	115.5 *	-26.50 *
MP Steam	HOT	175.0 *	174.0 *	21600.00 *	2.200e-006 *	165.5 *	115.5 *
HP Steam	HOT	250.0 *	249.0 *	21600.00 *	2.500e-006 *	240.5 *	165.5 *
Hot Oil	HOT	280.0 *	250.0 *	836.22 *	3.500e-006 *	275.5 *	240.5 *
Fired Heat (1000)	HOT	1000 *	400.0 *	399.60 *	4.249e-006 *	975.5 *	275.5 *
Fired Heat (2000)	HOT	2000 *	400.0 *	399.60 *	6.342e-006 *	1971 *	975.5 *
Very High Temperature	HOT	3000 *	2999 *	399.60 *	8.900e-006 *	2991 *	1971 *
Refrigerant 1 Generation	HOT	-24.00 *	-25.00 *	4680.00 *	-2.711e-006 *	-26.50 *	-41.50 *
Refrigerant 2 Generation	HOT	-39.00 *	-40.00 *	4680.00 *	-3.330e-006 *	-41.50 *	-65.50 *
Refrigerant 3 Generation	HOT	-64.00 *	-65.00 *	4680.00 *	-5.816e-006 *	-65.50 *	-103.5 *
Refrigerant 4 Generation	HOT	-102.0 *	-103.0 *	4680.00 *	-8.447e-006 *	-103.5 *	-273.1 *
Cooling Water	COLD	20.00 *	25.00 *	13500.00 *	2.125e-007 *	44.50 *	29.50 *
Air	COLD	30.00 *	35.00 *	399.60 *	1.000e-009 *	134.5 *	44.50 *
LP Steam Generation	COLD	124.0 *	125.0 *	21600.00 *	-1.890e-006 *	184.5 *	134.5 *
MP Steam Generation	COLD	174.0 *	175.0 *	21600.00 *	-2.190e-006 *	259.5 *	184.5 *
HP Steam Generation	COLD	249.0 *	250.0 *	21600.00 *	-2.490e-006 *	3000 *	259.5 *
Refrigerant 1	COLD	-25.00 *	-24.00 *	4680.00 *	2.739e-006 *	29.50 *	-21.50 *
Refrigerant 2	COLD	-40.00 *	-39.00 *	4680.00 *	3.364e-006 *	-21.50 *	-36.50 *
Refrigerant 3	COLD	-65.00 *	-64.00 *	4680.00 *	5.876e-006 *	-36.50 *	-62.50 *
Refrigerant 4	COLD	-103.0 *	-102.0 *	4680.00 *	8.531e-006 *	-62.50 *	-100.5 *
Very Low Temperature	COLD	-270.0 *	-269.0 *	4680.00 *	8.900e-006 *	-100.5 *	-267.5 *
Power	COLD	---	---	---	1.580e-005 *	---	---

4 CONCLUSIONS

At the end of this work, the following conclusion were drawn

1. Benzene, toluene and xylene was produced from liquefied petroleum gas (LPG) with purity of 68.83% for benzene, 89% for toluene and 92% for xylene. Other by-products such as heptane, octane, methane, hydrogen and fuel gas mixtures were also obtained.
2. The overall energy balance from ASPEN energy analyzer shows a power requirement of 5.33MW

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